

UNITARY SIMILARITY OF NONDEROGATORY MATRICES

YU. NESTERENKO

ABSTRACT. This paper is dedicated to the problem of verification of matrices for unitary similarity. For the case of nonderogatory matrices, we have been able to present the new solution for this problem based on geometric approach. The main advantage of this approach is stability with respect to errors in the initial upper triangular matrix. Since an upper triangular form is usually obtained by approximate methods (e.g. by QR algorithm), the mentioned advantage seems even more significant and allows us to propose the numerically stable and efficient method for verification of matrices for unitary similarity.

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1. INTRODUCTION

Matrices $A, B \in \mathbb{C}^{n \times n}$ are unitarily similar if a similarity transformation between them can be implemented using a unitary matrix U :

$$(1.1) \quad B = UAU^*.$$

A matrix $A \in \mathbb{C}^{n \times n}$ is called nonderogatory if its Jordan blocks have distinct eigenvalues. Equivalently, a matrix $A \in \mathbb{C}^{n \times n}$ is nonderogatory if and only if its characteristic polynomial and minimum polynomial coincide.

This paper concerns the verification of matrices for unitary similarity. Based on other authors' works concerning this problem, two basic approaches can be identified.

In the first, a complete system of matrix invariants under a unitary similarity transformation is constructed. In a sense, the final result in this direction is the Specht-Pearcy criterion (see [1, 2]), which reduces the question to verifying conditions of the form

$$(1.2) \quad \operatorname{tr} W(A, A^*) = \operatorname{tr} W(B, B^*)$$

for all words $W(s, t)$ of length at most $2n^2$. However, it seems that the number of words to be verified is strongly overestimated (see [3–6]). Moreover, this method cannot find a matrix generating a given unitary similarity.

The second approach is free of this shortcoming and consists of constructing a canonical form of matrices with respect to unitary similarity transformations. Inductive definitions of the canonical form of a matrix were proposed in [7–9], but it is hard to visualize the final canonical form. In more recently work [10] the authors, considered the set of nonderogatory matrix, constructed more visual canonical form.

In this work we propose the geometric approach to solving the problem for nonderogatory matrices. Given an arbitrary nonderogatory matrix, we construct a finite family of unitarily similar matrices for it (this family is called canonical). Whether or not two matrices are unitarily similar can be answered by verifying the intersection of their corresponding families. This method for unitary similarity verification has the significant advantage over the method [10] based on construction of the canonical form, it is stable with respect to errors in the initial matrix. This last aspect is discussed at the end of this paper.

While constructing a canonical family, we start from an upper triangular matrix form. Specifically, by the Schur theorem, any matrix $A \in \mathbb{C}^{n \times n}$ can be reduced

to such a form by using a unitary similarity transformation:

$$(1.3) \quad \Delta = \begin{bmatrix} \lambda_1 & \Delta_{12} & \Delta_{13} & \cdots & \Delta_{1n} \\ & \lambda_2 & \Delta_{23} & \cdots & \Delta_{2n} \\ & & \lambda_3 & & \\ & & & \ddots & \\ & & & & \lambda_n \end{bmatrix},$$

where $\lambda_1, \dots, \lambda_n$ are eigenvalues of the matrix with multiplicity in some fixed order. The next statement let us to restrict the set of unitary transformations while operating with a nonderogatory triangular matrices.

Lemma 1.1. *Let A be a nonderogatory complex $n \times n$ matrix, and let Δ be its upper triangular form with eigenvalues $\lambda_1, \dots, \lambda_n$ on the diagonal in some fixed order. Then the magnitudes of the elements Δ_{ij} , where $i < j$, are uniquely determined.*

Proof. Since the similar proposition for matrices with simple eigenvalues is known [8], we can consider the case of nonderogatory matrix with the single eigenvalue λ . Let Δ is obtained from A by unitary similarity transformation

$$(1.4) \quad \Delta = Q^* A Q$$

where $Q = (q_1 q_2 \dots q_n)$ is unitary matrix. Rewriting equation (1.4) as $AQ = Q\Delta$, one may see that q_1 is normalized eigenvector of the matrix A corresponding to the eigenvalue λ . Further,

$$(1.5) \quad Aq_2 = \Delta_{12}q_1 + \lambda q_2$$

, hence $(A - \lambda E)q_2 = 0$, i.e. q_2 is generalized eigenvector of A . Adding the condition of orthonormality of the pair q_1, q_2 , one obtains that q_2 is uniquely determined up to multiplication by a scalar of unit modulus. Continuing in the same vein, we can see that the matrix Q is uniquely determined up to multiplication by a diagonal unitary matrix, but such a transformations preserve the magnitudes of the off-diagonal elements of upper triangular form Q . Thus the lemma is proved.

Using the last lemma we can limit our consideration to studying the action of the group of unitary similarity transformations with diagonal matrices on the set of upper triangular matrices:

$$(1.6) \quad \Delta \mapsto X\Delta X^*, \quad X = \text{diag}(e^{i\psi_1}, \dots, e^{i\psi_{n-1}}, 1),$$

$$(1.7) \quad \{X\Delta X^*\}_{ij} = \begin{cases} \Delta_{ij}e^{i(\psi_i - \psi_j)} & i < j < n, \\ \Delta_{ij}e^{i\psi_i} & i < j = n, \\ \lambda_i & i = j, \\ 0 & i > j \end{cases}$$

(assuming the last diagonal entry of X is 1, we remove a scalar factor from X).

2. PRELIMINARY CONSTRUCTIONS

Let M denote the range of the parameters of the matrix

$$(2.1) \quad M = \{(r_{12}, \dots, r_{n-1,n}; \varphi_{12}, \dots, \varphi_{n-1,n}), \quad r_{ij}, \varphi_{ij} \in \mathbb{R}\},$$

and let M_r denote its restriction for fixed r_{ij} :

$$(2.2) \quad M_r = \{(r; \varphi) \in M : r_{ij} \text{ are fixed}\}.$$

The indices i and j run over the values $1 \leq i < j \leq n$ and are ordered lexicographically. For elements of M and M_r , several equivalent forms of notation are used:

$$(2.3) \quad (r_{12}, \dots, r_{n-1,n}; \varphi_{12}, \dots, \varphi_{n-1,n}) = (r; \varphi_{12}, \dots, \varphi_{n-1,n}) = (r; \varphi).$$

Looking ahead, r_{ij} and φ_{ij} will later play the role of absolute values and arguments of off-diagonal elements of Δ . Despite this geometric interpretation, no constraints are as yet imposed on r_{ij} and φ_{ij} and the indetermination of φ_{ij} at $r_{ij} = 0$ is ignored. At this stage, we work with the formally defined range M .

On M we introduce the family of transformations

$$(2.4) \quad X_\psi : (r; \varphi) \mapsto (r; \tilde{\varphi}),$$

$$(2.5) \quad \begin{aligned} \tilde{\varphi}_{ij} &= \varphi_{ij} + \psi_i - \psi_j, \quad 1 \leq i < j \leq n-1, \\ \tilde{\varphi}_{in} &= \varphi_{in} + \psi_i, \quad 1 \leq i \leq n-1. \end{aligned}$$

Each such a transformation is defined by a parameter vector $\psi = (\psi_1, \dots, \psi_{n-1}) \in \mathbb{R}^{n-1}$.

Consider a subset of matrices $K \subset M$ whose elements satisfy the system of equations

$$(2.6) \quad -\sum_{k=1}^{s-1} r_{ks} \varphi_{ks} + \sum_{k=s+1}^n r_{sk} \varphi_{sk} = 0, \quad s = 1, \dots, n-1.$$

The summation indices in (2.6) are visually described by the diagram

$$(2.7) \quad \begin{bmatrix} \lambda_1 & & & & * & & \\ & \ddots & & & * & & \\ & & \ddots & & * & & \\ & & & \ddots & \lambda_s & * & * \\ & & & & & \ddots & \\ & & & & & & \lambda_n \end{bmatrix}.$$

The reduction of an arbitrary matrix of M to a K form by applying a transformation X_ψ is reduced to finding the parameters of this transformation $\psi = (\psi_1, \dots, \psi_{n-1})$ by solving the system of linear equations

$$(2.8) \quad R(r)\psi = -b(r, \varphi)$$

with the symmetric matrix

$$(2.9) \quad \{R(r)\}_{ij} = \begin{cases} -r_{ij} & i < j, \\ \sum_{k=1}^{i-1} r_{ki} + \sum_{k=i+1}^n r_{ik} & i = j, \\ -r_{ji} & i > j \end{cases}$$

and with a righthand side that is linear in r and φ :

$$(2.10) \quad \begin{aligned} b(r, \varphi) &= (b_1(r, \varphi), \dots, b_{n-1}(r, \varphi)), \\ b_s(r, \varphi) &= -\sum_{k=1}^{s-1} r_{ks} \varphi_{ks} + \sum_{k=s+1}^n r_{sk} \varphi_{sk}, \quad s = 1, \dots, n-1. \end{aligned}$$

System (2.8) has some remarkable properties.

Theorem 2.1. (i) For any φ_{ij} and nonnegative r_{ij} , system (2.8) has a solution; i.e.,

$$(2.11) \quad -b(r, \varphi) \in \text{Im} R(r), \quad \forall \varphi_{ij}, \quad \forall r_{ij} \geq 0.$$

(ii) For all $r_{ij} \geq 0$, the determinant $\det R(r) \neq 0$ is nonzero if and only if the indices of the nonzero elements $r_{ij} > 0$ contain a collection $(ij)^1, \dots, (ij)^{n-1}$ such that the set $\{\psi_{i^p} - \psi_{j^p} \text{ (respectively } \psi_{i^p}, \text{ if } j^p = 0), \quad p = 1, \dots, n-1\}$ forms a linearly independent system of functions of variables $(\psi_1, \dots, \psi_{n-1})$.

(iii) Even if $\det R(r) = 0$ for some $r_{ij} \geq 0$, the solution of the equation $\psi = (\psi_1, \dots, \psi_{n-1})$ is such that the quantities

$$(2.12) \quad \begin{aligned} &r_{ij}(\psi_i - \psi_j), \quad 1 \leq i < j \leq n-1 \quad \text{and} \\ &r_{in}\psi_i, \quad 1 \leq i \leq n-1 \end{aligned}$$

are uniquely defined. This means that nonuniqueness in the definition of $\psi_i - \psi_j$ occurs if and only if $r_{ij} = 0$.

Proof. On the set M_r , we introduce the natural structure of a Euclidean space:

$$(2.13) \quad (r; \varphi^{(1)}) + (r; \varphi^{(2)}) = (r; \varphi_{12}^{(1)} + \varphi_{12}^{(2)}, \dots, \varphi_{n-1,n}^{(1)} + \varphi_{n-1,n}^{(2)}),$$

$$(2.14) \quad \alpha(r; \varphi) = (r; \alpha\varphi_{12}, \dots, \alpha\varphi_{n-1,n}), \quad \alpha \in \mathbb{R},$$

$$(2.15) \quad \langle (r; \varphi^{(1)}), (r; \varphi^{(2)}) \rangle = \sum_{1 \leq i < j \leq n} \varphi_{ij}^{(1)} \varphi_{ij}^{(2)}.$$

Then $K_r = M_r \cap K$ is a linear subspace of M_r that is orthogonal to all linear manifolds of the form

$$(2.16) \quad G_{r,\varphi} = \{(r; \varphi) + \sum_{1 \leq i < j \leq n-1} (\psi_i - \psi_j) r_{ij} \mathbb{I}_{ij} + \sum_{1 \leq i \leq n-1} \psi_i r_{in} \mathbb{I}_{in}, \quad \psi \in \mathbb{R}^{n-1}\},$$

$$(2.17) \quad \mathbb{I}_{ij} = (r; 0, \dots, 0, \overset{(ij)}{1}, 0, \dots, 0).$$

The dimensions of K_r and $G_{r,\varphi}$ depend on r , but their sum is a constant:

$$(2.18) \quad \dim K_r + \dim G_{r,\varphi} = \dim M_r.$$

In other words, in the Euclidean space M_r , the linear space K_r and the linear manifold $G_{r,\varphi}$ are mutually orthogonal and the sum of their dimensions is the complete one. This implies that they have a unique intersection point $(r; \varphi') = K_r \cap G_{r,\varphi}$. This intersection condition corresponds to the system of equations

$$(2.19) \quad R(r^2)\psi = -b(r, \varphi),$$

where r^2 denotes the vector

$$(2.20) \quad r^2 = (r_{12}^2, \dots, r_{n-1,n}^2).$$

In terms of ψ , the existence and uniqueness of an intersection point $(r; \varphi')$ means that system (2.19) is solvable with arbitrary φ_{ij} and r_{ij} and that the values

$$(2.21) \quad \begin{aligned} r_{ij}(\psi_i - \psi_j) &= f_{ij}, \quad 1 \leq i < j \leq n-1 \quad \text{and} \\ r_{in}\psi_i &= f_{in}, \quad 1 \leq i \leq n-1 \end{aligned}$$

are uniquely determined from it.

Assume that there exists an index set $(ij)^1, \dots, (ij)^{n-1}$ corresponding to the nonzero elements of $R(r^2)$ such that the set $\{\psi_{i^p} - \psi_{j^p} \text{ (respectively } \psi_{i^p}, \text{ if } j^p = 0), \quad p = 1, \dots, n-1\}$ forms a linearly independent system of functions of variables $(\psi_1, \dots, \psi_{n-1})$. Then a nondegenerate system of linear equations can be composed of relations (2.21) and $\psi = (\psi_1, \dots, \psi_{n-1})$ can be uniquely determined. Thus, under the conditions formulated, system (2.19) has a unique solution and, hence, $\det R(r) \neq 0$. The converse can be proved by contradiction.

The above results are extended to system (2.8) by making the substitution $r'_{ij} = r_{ij}^2 \geq 0$. The proof is complete.

Returning to the matrix Δ , we use Theorem 2.1 to construct the family of matrices that are unitarily similar to Δ .

With the help of the elements of Δ , we set up the system of linear equations

$$(2.22) \quad R(r)\psi = -b(r, \varphi + 2\pi m),$$

where r , φ , and m are defined as

$$(2.23) \quad r_{ij} = |\Delta_{ij}|, \quad \varphi_{ij} = \arg \Delta_{ij} - \pi, \quad m_{ij} \in \mathbb{Z}$$

Note that, despite the indetermination of φ_{ij} at $r_{ij} = 0$, the system of equations is uniquely defined.

Solving this system for $\psi = (\psi_1, \dots, \psi_{n-1})$, we construct the matrix $X\Delta X^*$, $X = \text{diag}(e^{i\psi_1}, \dots, e^{i\psi_{n-1}}, 1)$, which is unitarily similar to the original one. Again, if for some matrix Δ the parameter vector ψ is not determined uniquely from system (2.22), then, by Theorem 2.1, this nonuniqueness is such that the matrix $X\Delta X^*$ is uniquely determined.

The matrix generated by this procedure from Δ with the parameter vector $m = (m_{12}, \dots, m_{n-1,n})$ is denoted by $\mathcal{K}(\Delta, m)$.

3. ALGORITHM FOR CONSTRUCTING THE CANONICAL FAMILY

Now, we consider two nonderogatory upper triangular matrices $\Delta^{(1)}$ and $\Delta^{(2)}$ with identical sets of eigenvalues. The eigenvalues are assumed to be identically ordered on the matrix diagonals. For these matrices, we introduce $r_{ij}^{(1)}$, $\varphi_{ij}^{(1)}$ and $r_{ij}^{(2)}$, $\varphi_{ij}^{(2)}$ similar to (2.23). The matrices $\Delta^{(1)}$ and $\Delta^{(2)}$ are related by a unitary similarity transformation if and only if

- (i) $r_{ij}^{(1)} = r_{ij}^{(2)}$, $1 \leq i < j \leq n$ and
- (ii) there exist sets $(\psi_1, \dots, \psi_{n-1}) \in \mathbb{R}^{n-1}$ and $(k_{12}, \dots, k_{n-1,n}) \in \mathbb{Z}^{\frac{n(n-1)}{2}}$ such that, for indices (ij) corresponding $r_{ij}^{(1)} = r_{ij}^{(2)} > 0$, we have

$$(3.1) \quad \varphi_{ij}^{(1)} + 2\pi k_{ij}^{(1)} = \varphi_{ij}^{(2)} + 2\pi k_{ij}^{(2)} + \psi_i - \psi_j.$$

This implies that a unitary similarity of $\Delta^{(1)}$ and $\Delta^{(2)}$ is equivalent to $\mathcal{K}(C^{(1)}, k^{(1)}) = \mathcal{K}(C^{(2)}, k^{(2)})$ for some integer parameter vectors $k^{(1)} = (k_{12}^{(1)}, \dots, k_{n-1,n}^{(1)})$ and $k^{(2)} = (k_{12}^{(2)}, \dots, k_{n-1,n}^{(2)})$.

Let us represent the above criterion in an effective form. Define a subset $\mathbb{I} \subset \mathbb{Z}^{\frac{n(n-1)}{2}}$:

$$(3.2) \quad \mathbb{I} = \{k \in \mathbb{Z}^{\frac{n(n-1)}{2}} : k_{ij} = 0, \pm 1, \quad 1 \leq i < j \leq n-1, \\ k_{in} = 0, \quad 1 \leq i \leq n-1\}.$$

Theorem 3.1. *The matrices $\Delta^{(1)}$ and $\Delta^{(2)}$ are unitarily similar if and only if there exist vectors $k^{(1)}, k^{(2)} \in \mathbb{I}$ such that $\mathcal{K}(C^{(1)}, k^{(1)}) = \mathcal{K}(C^{(2)}, k^{(2)})$.*

Proof. Let $\Delta^{(1)}$ and $\Delta^{(2)}$ be unitarily similar and all their elements above the diagonal be nonzero. Then, as was shown above, there exist vectors $(\psi_1, \dots, \psi_{n-1}) \in \mathbb{R}^{n-1}$ and $k^{(1)}, k^{(2)} \in \mathbb{Z}^{\frac{n(n-1)}{2}}$ such that equalities (3.1) hold for all (ij) . We use them to make up the following linear combinations:

$$(3.3) \quad \varphi_{ij}^{(1)} - \varphi_{in}^{(1)} + \varphi_{jn}^{(1)} + 2\pi(k_{ij}^{(1)} - k_{in}^{(1)} + k_{jn}^{(1)}) = \\ = \varphi_{ij}^{(2)} - \varphi_{in}^{(2)} + \varphi_{jn}^{(2)} + 2\pi(k_{ij}^{(2)} - k_{in}^{(2)} + k_{jn}^{(2)}).$$

One may see that the ψ -dependent terms have canceled out. A feature of these linear combinations is that they are invariant under the action of transformations X_ψ on the linear space of vectors $\varphi = (\varphi_{12}, \dots, \varphi_{n-1,n})$. Moreover, these combinations form a basis in the subspace of linear functionals invariant under X_ψ .

Note that the conditions $\varphi_{ij}^{(s)} \in [-\pi, \pi)$ imply $\varphi_{ij}^{(s)} - \varphi_{in}^{(s)} + \varphi_{jn}^{(s)} \in (-3\pi, 3\pi)$, which in turn imply the following constraints on $k^{(1)}$ and $k^{(2)}$:

$$(3.4) \quad (k_{ij}^{(1)} - k_{in}^{(1)} + k_{jn}^{(1)}) - (k_{ij}^{(2)} - k_{in}^{(2)} + k_{jn}^{(2)}) = 0, \pm 1, \pm 2.$$

At the same time, the algorithm for deriving the matrix $\mathcal{K}(\Delta, 0)$ shows that the arguments of its elements are linearly expressed in terms of φ_{ij} :

$$(3.5) \quad \tilde{\varphi}_{ij} \in \mathcal{L}(\varphi_{12}, \dots, \varphi_{n-1,n}),$$

Moreover, these linear combinations must be invariant under X_ψ , so their form can be refined:

$$(3.6) \quad \tilde{\varphi}_{ij} \in \mathcal{L}(\{\varphi_{ij} - \varphi_{in} + \varphi_{jn}\}, \quad 1 \leq i < j \leq n-1).$$

Combining this with (3.4), we obtain the sufficiency of verifying the equalities $\mathcal{K}(\Delta^{(1)}, k^{(1)}) = \mathcal{K}(\Delta^{(2)}, k^{(2)})$ for $k^{(1)}, k^{(2)} \in \mathbb{I}$.

In the presence of zero elements above the diagonal of $\Delta^{(1)}$ and $\Delta^{(2)}$, the proposition is proved with slight modifications.

The finite set of matrices $\mathcal{K}(\Delta, k)$, $k \in \mathbb{I}$, that are unitarily similar to Δ is called the canonical family of the given matrix.

Thus, the following algorithm is proposed for verifying unitary similarity between nonderogatory matrices A and B with the same set of eigenvalues:

(i) Reduce these matrices to an upper triangular form with identically ordered eigenvalues on the diagonal to obtain matrices $\Delta^{(1)}$ and $\Delta^{(2)}$:

$$(3.7) \quad \Delta^{(1)} = U_1 A U_1^*, \quad \Delta^{(2)} = U_2 B U_2^*$$

(ii) For $\Delta^{(1)}$ and $\Delta^{(2)}$, construct their canonical families $\mathcal{K}(\Delta^{(1)}, k^{(1)})$ and $\mathcal{K}(\Delta^{(2)}, k^{(2)})$, $k^{(1)}, k^{(2)} \in \mathbb{I}$.

(iii) If these families intersect for some $k^{(1)}, k^{(2)} \in \mathbb{I}$ and

$$(3.8) \quad \mathcal{K}(\Delta^{(1)}, k^{(1)}) = X_1 \Delta^{(1)} X_1^*, \quad \mathcal{K}(\Delta^{(2)}, k^{(2)}) = X_2 \Delta^{(2)} X_2^*,$$

then the original matrices are similar and

$$(3.9) \quad B = U A U^*, \quad U = U_2^* X_2^* X_1 U_1.$$

Otherwise, they are not similar.

4. NUMERICAL STABILITY

The approach presented above significantly differs from earlier approaches to the problem studied. As a rule, different approaches (e.g. [8, 10]), based on the Schur upper triangular form, tried to create as many positive elements above the diagonal as possible. But such a property of a desired canonical form inevitably

leads to the form unstable with respect to errors in initial triangular form. One may observe the present effect on the next example:

$$(4.1) \quad A(\varepsilon) = \begin{bmatrix} 1 & i & i & i \\ 0 & 2 & i & i \\ 0 & 0 & 3 & \varepsilon \\ 0 & 0 & 0 & 4 \end{bmatrix},$$

where ε is a complex number. If the initially "strategy" of obtaining the greatest possible number of positive off-diagonal elements is to start with superdiagonal elements, then one can chose a $A(\varepsilon)$ arbitrary close (e.g. with respect to the Frobenius norm) to $A(0)$, but their canonical forms won't satisfy this property. The stability property seems even more significant due to the fact that usually an upper triangular form of a matrix is obtained by approximate methods (e.g. QR algorithm).

From the geometric point of view the constructed canonical family is the finite set of the ruled surfaces, such that an orbit of each nonderogatory matrix intersects each of them in a single point. The stability of this set of intersection points follows from the continuity of quantities (2.21) determined from system (2.22). The present property is of special interest in the context of the result obtained in [11]. Many ideas used by the author were taken from [12]. Specifically, a minimal continuous extension of a canonical Jordan form was constructed in [12]. Some of the results presented above are reflected in [13].

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YU. NESTERENKO, FACULTY OF COMPUTATIONAL MATHEMATICS AND CYBERNETICS, MOSCOW STATE UNIVERSITY, MOSCOW, RUSSIA

E-mail address: y_nesterenko@mail.ru